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This grant supported research in parameter estimation in distributed parameter systems, the research focused on theoretical and computational methods for estimation of unknown variable parameters in nonlinear partial differential equations. Also methods for estimating time delays in functional differential equations and boundary parameters in moving boundary problems were developed. Seven publications were produced under this grant, including "Estimation of

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→discontinuous coefficients and boundary parameters for hyperbolic systems" and
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PARAMETER ESTIMATION IN FUNCTIONAL & PARTIAL DIFF. EQNS.

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31 May 1989

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Summary

The investigator successfully obtained both theoretical and computational results for the estimation of unknown variable parameters in nonlinear functional and partial differential equations. Algorithms were developed to identify, from experimental data, unknown variable time delays appearing in functional differential equations and unknown variable coefficients (including boundary parameters and initial conditions) appearing in moving boundary problems. These algorithms require the discretization of infinite dimensional problems, in order to obtain computationally tractable finite dimensional approximating parameter estimation problems. The investigator proved theorems indicating that such approximating problems yield relevant information for the original problem of interest. The theoretical results were supplemented with numerical results obtained from several test problems.



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The general nature of the supported research was to develop methods for the problem of estimating parameters in a variety of applications. All of the problems considered involve models which are infinite dimensional (i.e. functional and partial differential equations). Many applications areas give rise to a differential equation model containing unknown parameters which one desires to estimate by fitting experimental data to the model equation. The general approach is to replace the original model equation with an approximating system of ordinary differential equations, and estimate parameters within this computationally tractable model. The aim, then, is to develop an approximation scheme which can be implemented efficiently, and also to prove that the "approximate parameter estimates" converge in some sense to a best-fit parameter for the original model.

Specifically the supported research, to be discussed in more detail below, pertains to the estimation of discontinuous, spatially varying coefficients in hyperbolic partial differential equations, the estimation of nonlinearities in parabolic differential equations, the estimation of nonconstant delays in functional differential equations and the estimation of parameters in moving boundary problems. In all cases, the goal is to develop computational methods and prove a corresponding convergence theorem for the parameter estimation problem.

The final revisions were made on a paper (now accepted for publication) representing research (joint work with P.K. Lamm of Michigan State University) on the estimation of discontinuous coefficients in hyperbolic partial differential equations ([1] of Publications arising under this period of support). This problem is motivated by seismic exploration. The response of the earth to a disturbance can be modeled in a simplified way by a one dimensional hyperbolic partial differential equation. The model equation will contain parameters representing physical characteristics of the earth, which are of great interest, but are often unknown. In general, these parameters will be spatially varying, as the earth is inhomogeneous, and possibly discontinuous. The problem then, is to identify these parameters based on observations of the earth's response to a surface disturbance.

Mathematically, one has data which corresponds to evaluations of the solution of the differential equation, and would like to find the parameters which provide a solution to the model equations which best fits this data. Thus, one must

obtain an estimate of a discontinuous function, including the location of the discontinuity. The general approach taken here is similar to that of others (eg., [1], [4]); the best-fit parameters are characterized as the minimizers of a least squares type fit to data. The original minimization problem is replaced by one in which the solution of an approximating system of ordinary differential equations has replaced the solution of the original partial differential equation. This approximate minimization problem is then solved iteratively on the computer. Both the model equations and the unknown parameters were approximated using splines. A computer program was written to implement the approximation scheme, and tested with several example problems. A convergence theory was simultaneously developed. This theory guarantees that the sequence of parameter estimates generated using the computationally attractive approximation scheme converges (in general, subsequentially) to best-fit parameters for the original problem. The new difficulty present in this problem is the unknown parameters are spatially varying, with an unknown location of discontinuity.

Additionally during this period, work was concluded on the estimation of nonlinear, state-dependent diffusion-type coefficients, and other nonlinearities in parabolic partial differential equations (joint with H.T. Banks of Brown University), resulting in a publication ([2] of Publications arising under this period of support). Such problems are of interest, for example, in ecology, in that these equations can be used to model insect population growth and dispersal. Some of this work was used with field data gathered in experiments performed by P. Kareiva to estimate unknown parameters occurring in a model for the interaction of ladybugs and aphids [3].

Similarly to the hyperbolic problem discussed above, the parameter estimation problem is posed as the minimization of a least-squares fit to data criterion which involves the solution of partial differential equations. Here, the model equations are a set of nonlinear coupled parabolic equations. The unknown parameters are state-dependent "diffusion" coefficients, and "reaction" nonlinearities (i.e., unknown nonlinear terms involving the states of the system). Again, similarly to the problem discussed above, both the states of the system and all nonconstant unknowns are approximated with splines. The difficult aspects of this problem are to prove a convergence theorem for this type of nonlinear system, and to develop numerical

schemes and convergence arguments for the estimation of nonlinear terms without assuming an *a priori* parametrization. This problem was successfully treated; computational packages were developed and tested on several numerical examples, and then applied to field data as mentioned earlier. In addition, a fairly general theory was developed (general in the scope of nonlinearities which can be estimated with these techniques).

The primary focus of the supported research has been, first, the development of numerical schemes and corresponding theory for the estimation of time- and state-dependent time delays in delay differential equations. Estimation of unknown constant delays in functional differential equations had been considered by many authors, for example, [2]. In the present work, the unknown parameter is a function, so that an additional level of approximation is required. Moreover, as the state space (on which the approximation algorithm is ultimately based) is intimately related to the size of the delay, a variable delay leads naturally to the consideration of a moving state-space. This introduces both theoretical and numerical complexities. We have been successful in developing both theoretical results and computational packages for this problem, and have generated several numerical test examples.

As with the constant delay problem, one can set up the delay differential equation abstractly, with states given by the current value of the solution in the first component, and the solution history (a function defined on the interval $[-\tau, 0]$, where τ is the delay) in the second component. Once τ is allowed to be variable (either time or state dependent), the second component begins to have a moving domain. The approximation technique used is similar to that of [2]; the interval $[-\tau, 0]$ is divided into subintervals, and the functional part of the state is approximated with splines (here, linear splines are used) defined on this grid. In the current research, since τ is variable, the approximations will move with time.

Three classes of nonconstant delay were considered: A delay which is an unknown function of time only, a delay which is determined through a differential equation which is coupled to the state equations, and a delay which is an unknown function of the state variable. A complete convergence theory has been developed for each of these three classes of delay. While the development of an estimation

algorithm and the numerical implementation was very similar for all types of delay, the theoretical treatment of each class was very different. Again, the approach in proving convergence is much like that of [2], in spirit, but there is the added difficulty of the moving approximations. While the definitions of the abstract differential equation, state spaces, norms, approximations, and projection operators are all formally similar, the fact of the variability in time (due to the variable delay) makes the convergence arguments more difficult. For example, the identity $\frac{d}{dt} \|x(t)\|^2 = 2 \langle x(t), \dot{x}(t) \rangle$ (an important tool in the convergence arguments of [2]) must now be modified to include a term accounting for the variation in time of the norm. This term contains the time derivative of τ . It is necessary for the convergence theorem to assume that τ satisfies $\dot{\tau} < 1$. This restriction is not unnatural in many applications problems, and can be implemented in a straightforward way in the case of $\tau = \tau(t)$. Ensuring that this condition holds for the other two cases of delay was a delicate, very technical problem, successfully resolved.

A further complication for the estimation of a variable delay is the secondary level of approximation necessary in order to estimate a functional unknown. The "true" function is replaced by an approximation, also based on splines. For the time-dependent delay case, if T is the final time of interest in the problem, then one subdivides the interval $[0, T]$ into equal subintervals, and defines splines (any order can be used; we have used both linear and cubic) on this grid. In the case of state dependent delay, one must choose, *a priori*, an estimate for the largest state value to be the width of the interval of approximation. One then estimates a spline-based approximate delay function. This secondary level of approximation is much like that used for the estimation of functional coefficients in partial differential equations (see for example [4], and [1] of Publications arising under this period of support), and that used for the estimation of state-dependent parameters in nonlinear partial differential equations (as in [2] of Publications arising under this period of support).

In summary, a spline-based approximation scheme has been developed for the estimation of variable delays in nonlinear functional differential equations. The types of variable delays one encounters fall naturally into three classes (time-dependent, implicitly state-dependent, and explicitly state-dependent). The scheme

can also be used to estimate other unknown parameters, however this is a straightforward modification of the work in [2], and is not new. A convergence theorem has been proved for each of the three types of variable delay. It says essentially that if one restricts the search for the unknown parameters to certain parameter sets, then one is guaranteed that performing the minimization using approximations will yield a sequence of parameter estimates that converge subsequentially to a best-fit parameter for the original model equations. The constraint set within which one must search is not unduly restrictive; it is common in parameter estimation problems to require that the constraint set be compact. We require compactness conditions and we additionally require the $\hat{\tau}$ be bounded below one and have some lower bound. Again, this has an interpretation (causality) which is not unnatural in many applications. Finally, we have developed a computational package and used it to perform several numerical test examples. All of the above will appear in [4] of Publications arising under this period of support, and some examples and a brief discussion of the results can be found in [3] of Publications arising under this period of support.

The second major goal of the sponsored research has been to extend the ideas discussed above to the problem of estimating parameters in moving boundary problems. Here, one has a parabolic partial differential equation defined on a domain which moves in time. Thus, since a common approach is to approximate the solution of a partial differential equation using splines defined on a partition of the domain, it is natural to use approximations which move in time, just as was done with the delay equations. In fact, the theoretical arguments become much easier if one first transforms the problem (via a straightforward change of variables) to a problem on a fixed spatial domain (the dynamics of this transformed problem are then more complicated, and nonlinear, even if the original dynamics were linear). We began our investigations by setting up moving approximations, but then performed the theoretical analysis on the fixed-domain problem. Either way, (i.e., whether one discretizes the original problem with moving elements, or transforms the problem to the fixed domain first), one ultimately obtains the same numerical scheme.

The moving boundary problems we have considered are characterized by the fact that the movement of the boundary is determined by an equation involving the

state variable. Thus, such problems are formulated as a coupled system of a parabolic partial differential equation (for the state) and an ordinary differential equation (for the location of the boundary). It is this coupling which makes these problems nonlinear. It is through this coupling that we have defined a class of moving boundary problems which are amenable to theoretical analysis. The class of problems for which we have obtained our convergence result is briefly characterized by the following. After the change of variables (let $U(t,y)$ represent the new state variable, with the new spatial variable $y \in [0,1]$), we write the dynamics for the movement of the boundary as $\dot{s}(t) = \mathcal{F}(t,U,s)$ where $s(t)$ represents the location of the boundary at time t . The class of problems which we have considered requires essentially that \mathcal{F} be continuous in U in the $H^1[0,1]$ topology. For this class of problems, we have developed an approximation scheme, and proved a convergence theorem of the desired form (i.e., by solving the parameter estimation problem using the approximate model equations, one obtains a sequence of parameter estimates which converges subsequentially to a best-fit parameter for the original model equations). These results are the subject of [5, 6, 7] of Publications arising under this period of support. It is interesting to note that our numerical scheme has been successful (in test numerical examples) for estimating parameters in model equations which do not fit into our theoretical framework (such as the Stefan problem and the Oxygen Diffusion problem).

As an example of a moving boundary problem which fits into the theoretical framework of this research, consider the absorption of pollutants on activated carbon particles [5]. The model equation for the full problem is complicated; if one considers only the activity surrounding a single carbon particle, then one can derive a model equation which is a diffusion equation with a moving boundary. The moving boundary arises due to the fact that a bacterial layer forms on the outside of the carbon particle. In order for the pollutant to bind onto the carbon particle, it must first pass through this layer. As the pollutant diffuses through the bacterial layer, some of it is used by the bacteria as nutrient. The width of the bacterial layer changes in time as the bacteria grows (due to feeding on the pollutant) and is lost (due to death, shearing off into the surrounding fluid, etc.).

A simple model is thus a diffusion equation with standard boundary conditions, but a changing spatial domain, $[0, s(t)]$, where $s(t)$ measures the width of the biofilm layer. To make the problem well-posed, an additional condition is

specified. This condition is of the form $\dot{s}(t) = \int_0^{s(t)} F(t,x,u) dx$, where u represents the concentration of the pollutant and F is a nonlinear function describing the dynamics of bacterial activity (i.e., F will describe how the bacteria uses pollutant, rate of loss, etc.). After the change of variables to fixed domain, this equation has the form $\dot{s}(t) = s(t) \int_0^1 \tilde{F}(t,y,U) dy$. Under physically reasonable assumptions on F , it has been shown that this equation satisfies the assumptions we require for our theory. In [6] and [7] of Publications arising under this period of support, more examples of applications satisfying our theoretical assumptions can be found.

Once we transformed the problem to the fixed domain, our approximations were performed in a straightforward manner. Approximating the state variable U is standard (see, eg., [1]); we then coupled the resulting system of ordinary differential equations (the solution of which gives the approximate, U^N) with the given ordinary differential equation describing the dynamics for s . The original dynamics for s involve U ; we solved for an approximation s^N , using the given equation with U^N substituted for U . Our key convergence result then involves a statement of the form: For any convergent sequence of parameters $q^N \rightarrow q$, it follows that $(U^N(q^N), s^N(q^N)) \rightarrow (U(q), s(q))$ in $H^0(0,1) \times \mathbb{R}$. This result was technically difficult to argue, but once established, it allowed us to argue that our parameter estimates obtained under the approximations converge subsequentially to a best-fit for the problem of interest.

In addition to the moving boundary problem described above, the Stefan problem (see, eg., [6]) and a problem of Oxygen Diffusion (eg., [7]) have also been considered. The numerical package mentioned above has been modified to perform several test examples of parameter estimation problems within these types of equations (some of these examples appear in [3] and in [7] of Publications arising under this period of support), however the convergence theory is more difficult due to the fact that the extra condition (like \dot{s} in the problem above) involves a pointwise evaluation of a derivative of the state, u for the Stefan problem, and an extra condition on u (rather than an equation for \dot{s}) in the Oxygen Diffusion problem. Current investigations center on proving a convergence theorem for this type of moving boundary problem.

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Interactions:

During the 1986-1987 academic year, the investigator gave seminar talks about the estimation of time- and state-dependent delays at North Carolina State University, Duke University, and the University of North Carolina at Chapel Hill.

In July of 1987, the investigator was invited to participate in the Workshop for Control and Identification at ICASE, NASA Langley Research Center, where she was a Scientific Consultant. There she discussed her work on estimation of delays in functional differential equations and parameter estimation in moving boundary problems.

In October of 1987 the investigator gave a contributed presentation entitled "A Numerical Method for Parameter Estimation in Moving Boundary Problems" at the SIAM 35th Anniversary Meeting in Denver, CO.

In December of 1987 the investigator gave an invited lecture entitled "Time-Dependent Approximation Schemes for Some Problems of Parameter Estimation in Distributed Systems", at the 26th IEEE Conference on Decision and Control in Los Angeles, CA.

In July of 1988 the investigator gave a contributed presentation entitled "A Numerical Method for the Estimation of Variable Time Delays with Applications to Biology" at the SIAM Annual Meeting in Minneapolis, MN.

In August of 1988 the investigator attended the Brown/INRIA NSF Workshop on Control and Identification for Distributed Systems, at Brown University, where she gave a talk entitled "Parameter Estimation in Moving Boundary Problems".

In September of 1988 the investigator gave a contributed presentation entitled "A Numerical Method for Parameter Estimation in Moving Boundary Problems" at the Virginia Tech-ICAM Conference on Numerical Solutions of Partial Differential Equations, held at Virginia Polytechnic Institute in Blacksburg, VA..

During the 1988-1989 academic year, the investigator gave several seminar talks about the estimation of variable parameters in Moving Boundary problems, at North Carolina State University, and the University of North Carolina at Chapel Hill.

In December of 1988 the investigator gave an invited lecture entitled "Parameter Estimation in Moving Boundary Problems", at the 27th IEEE Conference on Decision and Control in Austin, TX.